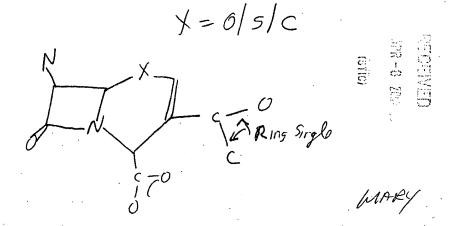
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STEREO ATTRIBUTES: NONE

L3 8 SEA FILE=REGISTRY SSS FUL L1

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8 ANSWERS

SEARCH TIME: 00.00.03

L3 ANSWER 1 OF 8 REGISTRY COPYRIGHT 2002 ACS 395661-06-0 REGISTRY RN 5-Thia-1-azabicyclo[4.2.0]oct-3-ene-2-carboxylic acid, CN 8-oxo-7-[(phenylacetyl)amino]-3-[(2R)-tetrahydro-2-furanyl}-, (4-methoxyphenyl)methyl ester, (2R,6R,7R)- (9CI) (CA INDEX NAME) FS STEREOSEARCH C27 H28 N2 O6 S MFSR CA ·LC STN Files: CA, CAPLUS

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:151036 Process for the preparation of cephalosporin compounds and their intermediates. Burton, George; Best, Desmond John; Gasson, Brian Charles; Osborne, Neal Frederick; Walker, Graham (Pfizer Inc., USA). Eur. Pat. Appl. EP 1178049 A1 20020206, 22 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO. (English). CODEN: EPXXDW. APPLICATION: EP 2001-306325 20010723. PRIORITY: GB 2000-19124 20000803.

GI

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB A process for prepg. cephalosporins I (R1 = H, OMe, formamido; R2 = acyl; CO2R3 = carboxy group or CO2- or readily removable carboxy protecting group; R4 = H, or up to four substituents from alkyl, alkenyl, alkynyl, alkoxy, halogen, amino, alkyl(acyl)amino, CO2R, CONR2, SO2NR2 (R = H, C1-6 alkyl), aryl, heterocycle, etc.; X = S, SO, SO2, O, CH2; m = 1-2; dotted lines indicate a 2- or 3-cephem system) was accomplished via the cyclization of II. Thus the 3-(R and S)-tetrahydrofuran-2-yl-2-em compds. III were prepd. and the S isomer was converted to the 3-(S)-tetrahydrofuran-2-yl-3-em III in several steps.
- L3 ANSWER 2 OF 8 REGISTRY COPYRIGHT 2002 ACS
- RN 395661-05-9 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-3-ene-2-carboxylic acid, 8-oxo-7-[(phenylacetyl)amino]-3-[(2S)-tetrahydro-2-furanyl]-, (4-methoxyphenyl)methyl ester, (2R, 6R, 7R)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF . C27 H28 N2 O6 S
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:151036 Process for the preparation of cephalosporin compounds and their intermediates. Burton, George; Best, Desmond John; Gasson, Brian Charles; Osborne, Neal Frederick; Walker, Graham (Pfizer Inc., USA). Eur. Pat. Appl. EP 1178049 A1 20020206, 22 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO. (English). CODEN: EPXXDW. APPLICATION: EP 2001-306325 20010723. PRIORITY: GB 2000-19124 20000803.

GΙ

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB A process for prepg. cephalosporins I (R1 = H, OMe, formamido; R2 = acyl; CO2R3 = carboxy group or CO2- or readily removable carboxy protecting group; R4 = H, or up to four substituents from alkyl, alkenyl, alkynyl, alkoxy, halogen, amino, alkyl(acyl)amino, CO2R, CONR2, SO2NR2 (R = H, C1-6 alkyl), aryl, heterocycle, etc.; X = S, SO, SO2, O, CH2; m = 1-2; dotted lines indicate a 2- or 3-cephem system) was accomplished via the cyclization of II. Thus the 3-(R and S)-tetrahydrofuran-2-yl-2-em compds. III were prepd. and the S isomer was converted to the 3-(S)-tetrahydrofuran-2-yl-3-em III in several steps.
- L3 ANSWER 3 OF 8 REGISTRY COPYRIGHT 2002 ACS
- RN 395660-98-7 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-3-ene-2-carboxylic acid, 8-oxo-7-[(phenylacetyl)amino]-3-[(2R)-tetrahydro-2-furanyl]-, diphenylmethyl ester, (2R,6R,7R)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C32 H30 N2 O5 S
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:151036 Process for the preparation of cephalosporin compounds and their intermediates. Burton, George; Best, Desmond John; Gasson, Brian Charles; Osborne, Neal Frederick; Walker, Graham (Pfizer Inc., USA). Eur. Pat. Appl. EP 1178049 A1 20020206, 22 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO. (English). CODEN: EPXXDW. APPLICATION: EP 2001-306325 20010723. PRIORITY: GB 2000-19124 20000803.

GI

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB A process for prepg. cephalosporins I (R1 = H, OMe, formamido; R2 = acyl; CO2R3 = carboxy group or CO2- or readily removable carboxy protecting group; R4 = H, or up to four substituents from alkyl, alkenyl, alkynyl, alkoxy, halogen, amino, alkyl(acyl)amino, CO2R, CONR2, SO2NR2 (R = H, C1-6 alkyl), aryl, heterocycle, etc.; X = S, SO, SO2, O, CH2; m = 1-2; dotted lines indicate a 2- or 3-cephem system) was accomplished via the cyclization of II. Thus the 3-(R and S)-tetrahydrofuran-2-yl-2-em compds. III were prepd. and the S isomer was converted to the 3-(S)-tetrahydrofuran-2-yl-3-em III in several steps.
- L3 ANSWER 4 OF 8 REGISTRY COPYRIGHT 2002 ACS
- RN 395660-97-6 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-3-ene-2-carboxylic acid, 8-oxo-7-[(phenylacetyl)amino]-3-[(2S)-tetrahydro-2-furanyl]-, diphenylmethyl ester, (2R,6R,7R)- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C32 H30 N2 O5 S
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:151036 Process for the preparation of cephalosporin compounds and their intermediates. Burton, George; Best, Desmond John'; Gasson, Brian Charles; Osborne, Neal Frederick; Walker, Graham (Pfizer Inc., USA). Eur. Pat. Appl. EP 1178049 A1 20020206, 22 pp. DESIGNATED STATES: R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO. (English). CODEN: EPXXDW. APPLICATION: EP 2001-306325 20010723. PRIORITY: GB 2000-19124 20000803.

GΙ

- * STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT *
- AB A process for prepg. cephalosporins I (R1 = H, OMe, formamido; R2 = acyl; CO2R3 = carboxy group or CO2- or readily removable carboxy protecting group; R4 = H, or up to four substituents from alkyl, alkenyl, alkynyl, alkoxy, halogen, amino, alkyl(acyl)amino, CO2R, CONR2, SO2NR2 (R = H, C1-6 alkyl), aryl, heterocycle, etc.; X = S, SO, SO2, O, CH2; m = 1-2; dotted lines indicate a 2- or 3-cephem system) was accomplished via the cyclization of II. Thus the 3-(R and S)-tetrahydrofuran-2-yl-2-em compds. III were prepd. and the S isomer was converted to the 3-(S)-tetrahydrofuran-2-yl-3-em III in several steps.
- L3 ANSWER 5 OF 8 REGISTRY COPYRIGHT 2002 ACS
- RN 191919-05-8 REGISTRY
- CN 5-Thia-1-azabicyclo[4.2.0]oct-3-ene-2-carboxylic acid, 8-oxo-7-[(phenylacetyl)amino]-3-(tetrahydro-2-furanyl)-, diphenylmethyl ester, [2R-(2.alpha.,6.alpha.,7.beta.)]-[partial]- (9CI) (CA INDEX NAME)
- FS STEREOSEARCH
- MF C32 H30 N2 O5 S
- SR CA
- LC STN Files: CA, CAPLUS

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 127:81262 Cycloadditions of Cephalosporins. A Comprehensive Study of the Reaction of Cephalosporin Triflates with Olefins, Acetylenes, and Dienes To Form [2 + 2] and [4 + 2] Adducts. Elliott, Richard L.; Nicholson, Neville H.; Peaker, Fiona E.; Takle, Andrew K.; Richardson, Christine M.; Tyler, John W.; White, Janet; Pearson, Michael J.; Eggleston, Drake S.; Haltiwanger, R. Curtis (New Frontiers Science Park (North), SmithKline Beecham Pharmaceuticals, Harlow/Essex, CM19 5AW, UK). J. Org. Chem., 62(15), 4998-5016 (English) 1997. CODEN: JOCEAH. ISSN: 0022-3263. Publisher: American Chemical Society.

AΒ Novel polycyclic cephalosporins are formed by the reaction of cephalosporin triflates with various unsatd. compds. in the presence of Hunigs base. 2,3-Fused cyclobutane and cyclobutene cephems are obtained with olefins and acetylenes, resp., whereas [4 + 2] cycloadducts are obtained with furan. The reaction has been rationalized by invoking the intermediacy of a strained 6-membered cyclic allene. The allene undergoes an orbital symmetry allowed concerted .pi.2s + .pi.2a cycloaddn. with olefins and acetylenes and a .pi.4s + .pi.2s cycloaddn. with furan. The regiochem. of the [2 + 2] cycloadducts is independent of the substitution of the unsatd. component and of the oxidn. state of the cephalosporin sulfur atom. However in the case of the [4 + 2] adducts, the sulfur oxidn. state dets. the regiochem. of the addn. Carbacephalosporins also participate in this reaction with olefins but require a stronger base such as DBU. Thus the reaction described provides a facile, one-step procedure for the prodn. of a rich variety of novel polycyclic cephalosporins.

L3 ANSWER 6 OF 8 REGISTRY COPYRIGHT 2002 ACS

RN 146451-30-1 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-3-ene-2-carboxylic acid, 3-[3-(ethoxycarbonyl)-4,5-dihydro-5-isoxazolyl]-8-oxo-7-[(phenylacetyl)amino]-, (4-methoxyphenyl)methyl ester, [2R-[2.alpha.,3(R*),6.alpha.,7.beta.]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C29 H29 N3 O8 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 118:212718 Synthesis and activity of 3-(isoxazolin-5-yl)- and 3-(isoxazol-4-yl)cephalosporins. Koyama, Yoshiyuki; Huang, Shyh Pyng; Ikeda, Daishiro; Kondo, Shinichi; Takeuchi, Tomio (Inst. Microb. Chem., Tokyo, 141, Japan). J. Antibiot., 45(12), 1930-8 (English) 1992. CODEN: JANTAJ. ISSN: 0021-8820.

GI

AB The 1,3-dipolar cycloaddn. of nitrile oxides with 3-vinylcephalosporin I (R = H, Me) provided diastereomeric isomers of 3-(isoxazolin-5-yl)cephalosporin II (R = H, Me; R1 = Me, CONH2, CO2Et). Similarly cycloaddn. of nitrile oxides with 3-(dimethylaminovinyl)cephalosporin gave 3-(isoxazol-4-yl)cephalosporins. These semisynthetic cephalosporins with an aminothiazole in the C-7 side chain showed moderate antibacterial activities.

L3 ANSWER 7 OF 8 REGISTRY COPYRIGHT 2002 ACS

RN 142369-30-0 REGISTRY
CN 5-Thia-1-azabicyclo[4.2.0]oct-3-ene-2-carboxylic acid,
8-oxo-7-[(phenylacetyl)amino]-3-(tetrahydro-2-furanyl)-, diphenylmethyl
ester, [6R-(6.alpha.,7.beta.)]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C32 H30 N2 O5 S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 116:255397 Preparation of 3-tetrahydrofurylcephem-3-carboxylates and analogs as antibiotics. Bateson, John Hargreaves; Burton, George; Fell, Stephen Christopher Martin (Beecham Group PLC, UK). PCT Int. Appl. WO 9201696 A1 19920206, 147 pp. DESIGNATED STATES: W: AU, CA, CS, FI, HU, JP, KR, NO, PL, US; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1991-GB1228 19910722. PRIORITY: GB 1990-16189 19900724; GB 1991-9540 19910502.

GI For diagram(s), see printed CA Issue.

AB Title compds. (I; R1 = H, MeO, HCONH; R2 = acyl; R3 = H, neg. charge, carboxy-protective group; R4 = .ltoreq.4 substituents selected from alkyl, alkenyl, OH, halo, alkoxy, etc.; X = O, CH2, SOn; n= 0-2; m = 1, 2) were prepd. Thus, Na 2-(2-tritylaminothiazol-4-yl)-2-(Z)-trityloxyiminoacetate was condensed with tert-butyl (6R, 7R)-7-amino-3-[(R)-tetrahydrofuran-2-yl]ceph-3-em-4-carboxylate to give, after deprotection, (6R, 7R)-7-[2-(2-aminothiazol-4-yl)-2-(Z)-hydroxyiminoacetamido]-3-[(RS)-tetrahydrofuran-2-yl]ceph-3-em-4-carboxylic acid which had MIC of 0.50 and 0.25 .mu.g/mL against Escherichia coli (NCTC 1048) and Staphylococcus aureus (Oxford), resp.

L3 ANSWER 8 OF 8 REGISTRY COPYRIGHT 2002 ACS

RN 131528-26-2 REGISTRY

CN 5-Thia-1-azabicyclo[4.2.0]oct-3-ene-2-carboxylic acid, 3-[3-(ethoxycarbonyl)-4,5-dihydro-5-isoxazolyl]-8-oxo-7-[(phenylacetyl)amino]-, (4-methoxyphenyl)methyl ester, [6R-[3(R*),6.alpha.,7.beta.]]- (9CI) (CA INDEX NAME)

FS STEREOSEARCH

MF C29 H29 N3 O8 S

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 114:61749 Synthesis of 3-isoxazolidinylcephalosporin and its analogs via 1,3-dipolar cycloaddition of 3-vinylcephem. Huang, Shyh Pyng; Ikeda, Daishiro; Koyama, Yoshiyuki; Kondo, Shinichi (Inst. Microb. Chem., Tokyo, 141, Japan). Synlett (7), 391-2 (English) 1990. CODEN: SYNLES.

AB Cephalosporins I [RR1 = NMeCH2CH2, N+Me2CH2CH2 I-, N:C(CO2Et)CH2] were obtained by treating vinylcephem with CH2:N(O)Me or EtO2CCNO resp.

Transacylation gave the cephalosporin II which inhibited Escherichia coli K-12 C600 at 0.05 .mu.g/mL.

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